

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
 Data File : BP018971.D
 Acq On : 20 Dec 2023 21:09
 Operator : MA/JU
 Sample : 05894-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BH3K5

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018971.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.675	96	100	115	rBV	137777	210049	0.35%	0.208%
2	6.999	660	665	673	rVB	110899	175208	0.29%	0.173%
3	7.163	687	693	706	rVB	454486	706349	1.17%	0.699%
4	7.357	718	726	736	rBV	435843	679951	1.13%	0.673%
5	7.822	797	805	816	rBV	475502	754113	1.25%	0.747%
6	8.540	920	927	937	rBV	346830	553759	0.92%	0.548%
7	8.987	994	1003	1013	rBV	551106	893314	1.48%	0.884%
8	9.704	1119	1125	1134	rBV	436244	712636	1.18%	0.706%
9	10.246	1208	1217	1234	rBV	641555	1125457	1.87%	1.114%
10	10.616	1273	1280	1287	rBV	587188	987436	1.64%	0.978%
11	10.763	1297	1305	1318	rBV	440003	780433	1.29%	0.773%
12	13.875	1828	1834	1850	rBV	1385877	1882360	3.12%	1.864%
13	14.151	1871	1881	1894	rBV	1555848	2293279	3.80%	2.270%
14	14.457	1926	1933	1948	rBV	920501	1408319	2.34%	1.394%
15	14.681	1966	1971	1983	rBV	76651	161546	0.27%	0.160%
16	15.451	2094	2102	2108	rBV	2069367	2924329	4.85%	2.895%
17	15.575	2117	2123	2132	rBV	600892	847852	1.41%	0.839%
18	17.098	2363	2382	2386	rBV	17047695	60299779	100.00%	59.700%
19	17.175	2391	2395	2397	rVV2	178367	258221	0.43%	0.256%
20	17.210	2397	2401	2410	rVV	1195406	1682064	2.79%	1.665%
21	17.310	2412	2418	2429	rVB2	2227794	3217117	5.34%	3.185%
22	18.098	2548	2552	2561	rBV	118978	188518	0.31%	0.187%
23	19.033	2707	2711	2716	rBV	222127	258266	0.43%	0.256%
24	19.192	2734	2738	2741	rBV	43233	60303	0.10%	0.060%
25	19.333	2759	2762	2768	rBV2	63340	82638	0.14%	0.082%
26	19.551	2793	2799	2805	rBV	3233428	4358093	7.23%	4.315%
27	21.298	3091	3096	3103	rBV	1859536	2388888	3.96%	2.365%
28	21.392	3108	3112	3117	rVV	650268	768741	1.27%	0.761%
29	22.527	3301	3305	3312	rVB	495956	714008	1.18%	0.707%
30	23.515	3465	3473	3486	rVB	2735319	5512667	9.14%	5.458%
31	23.663	3492	3498	3506	rVB	1332095	2633578	4.37%	2.607%
32	23.927	3537	3543	3551	rVB	746882	1484957	2.46%	1.470%

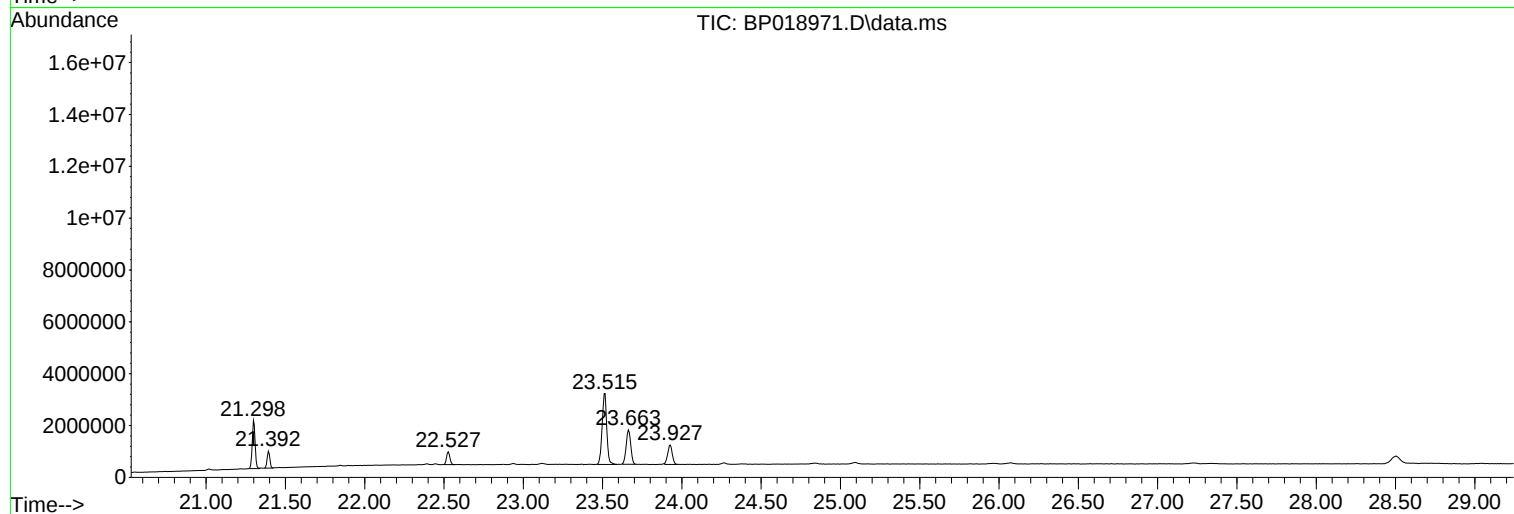
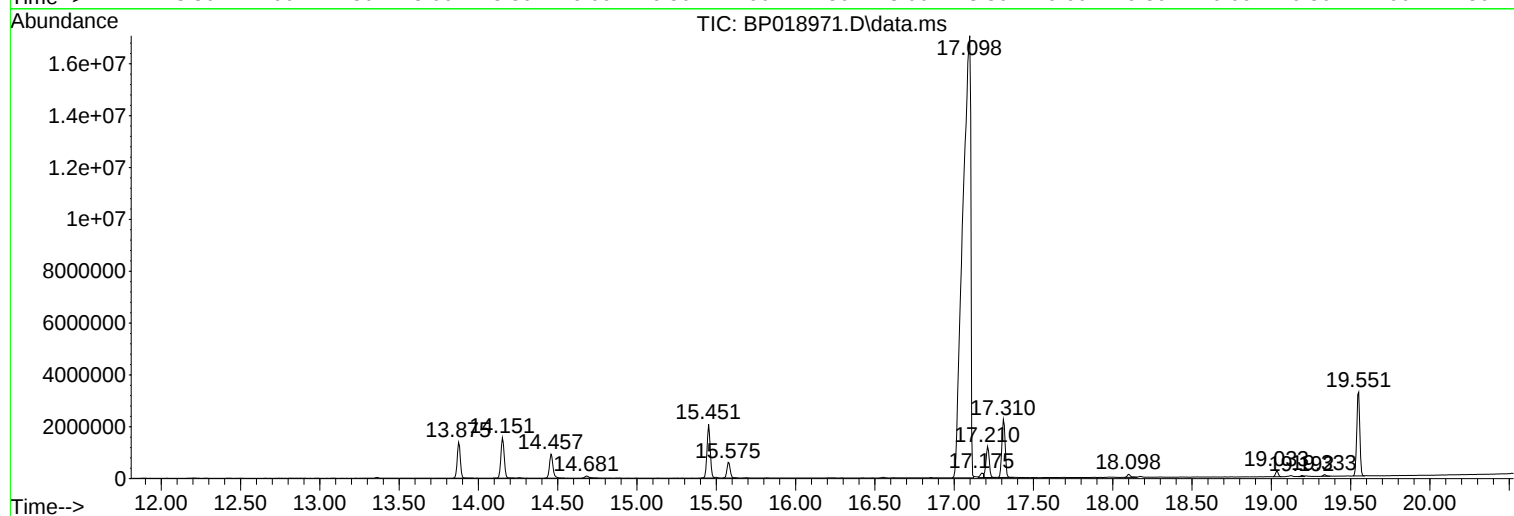
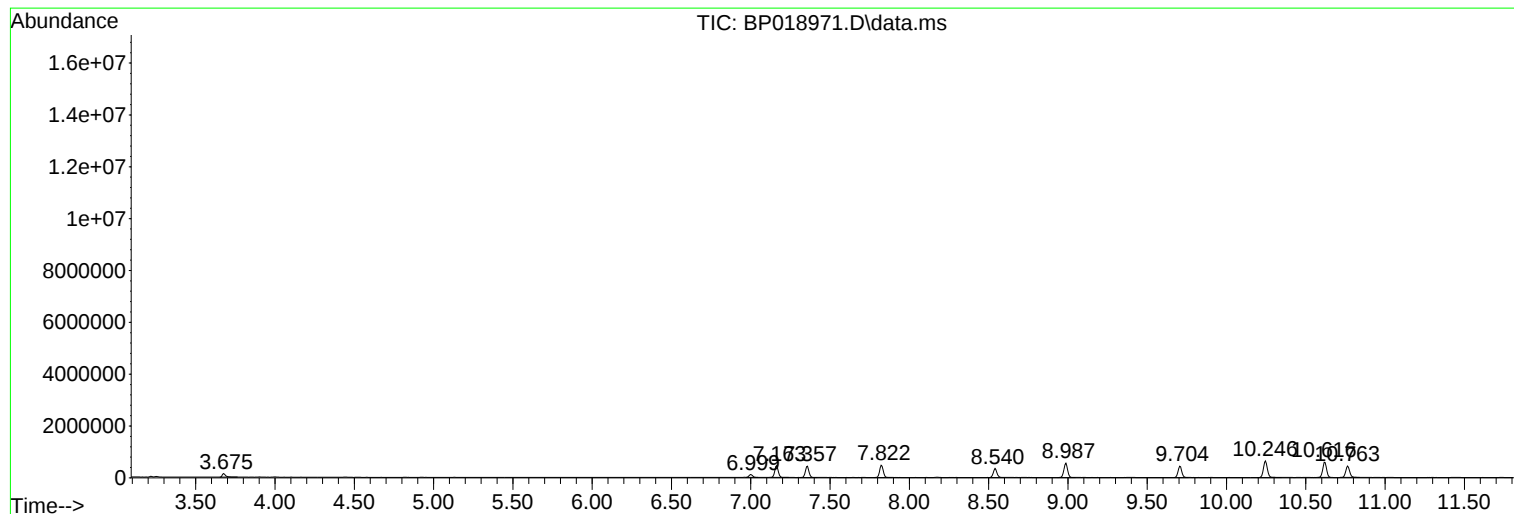
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P



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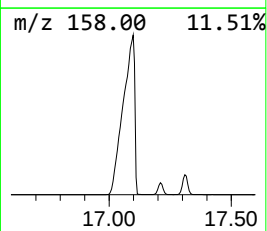
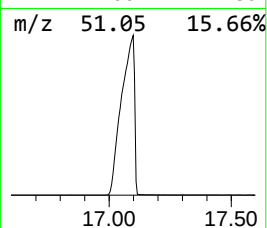
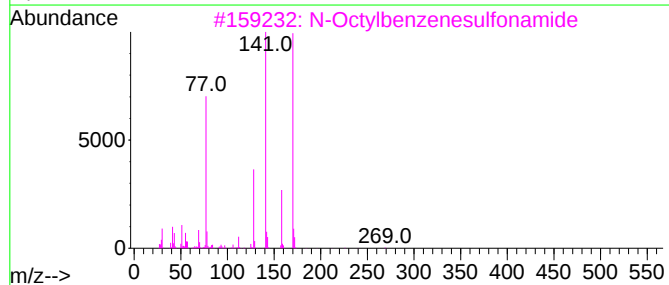
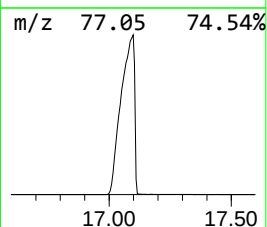
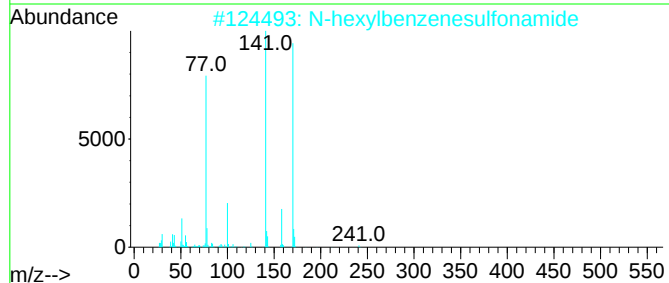
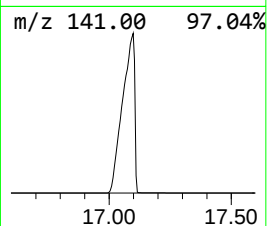
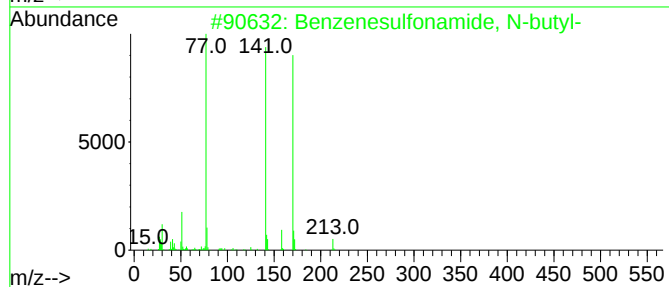
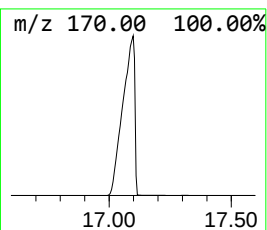
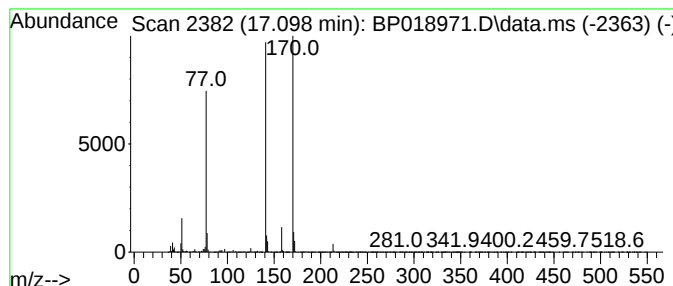
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzenesulfonamide, N-butyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.098	716.97 ng/ul	60299800	Phenanthrene-d10	17.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	95
2			N-hexylbenzenesulfonamide	241	C12H19NO2S	007250-80-8	80
3			N-Octylbenzenesulfonamide	269	C14H23NO2S	016358-32-0	74
4			2-propenoic acid, 2-methyl-, 2-[...]	269	C12H15NO4S	1000401-71-8	64
5			2-Fluoro-6-hydroxypyridine, tert...	227	C11H18FNOSi	1000493-97-6	47



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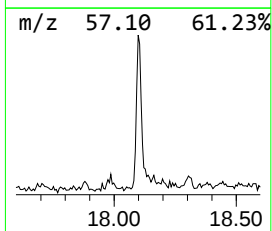
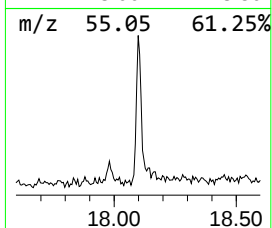
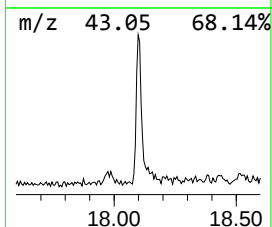
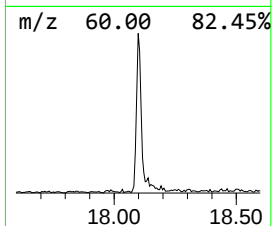
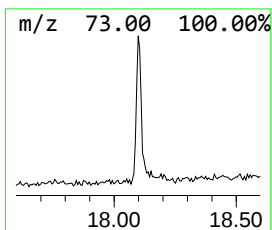
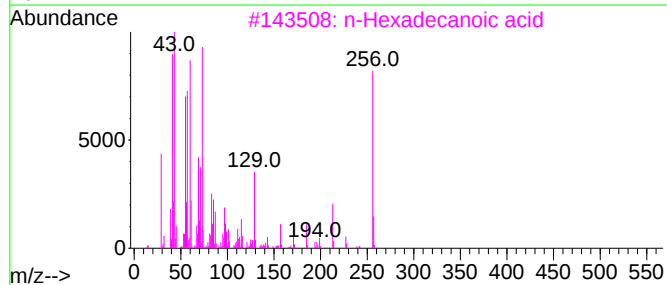
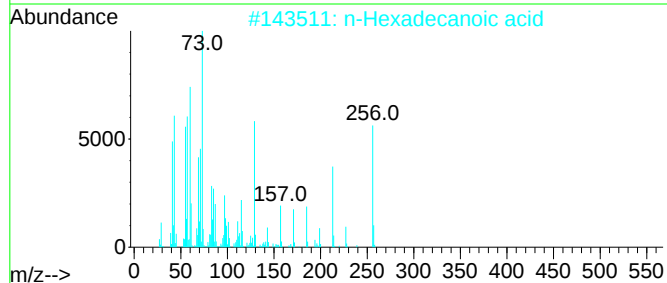
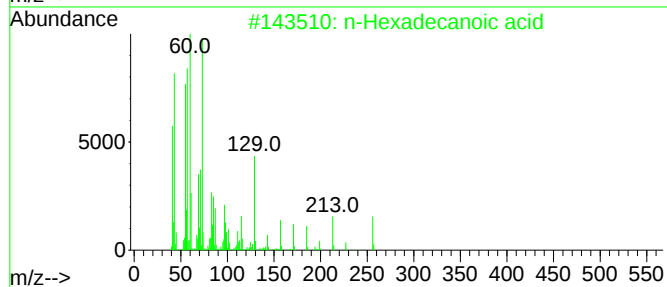
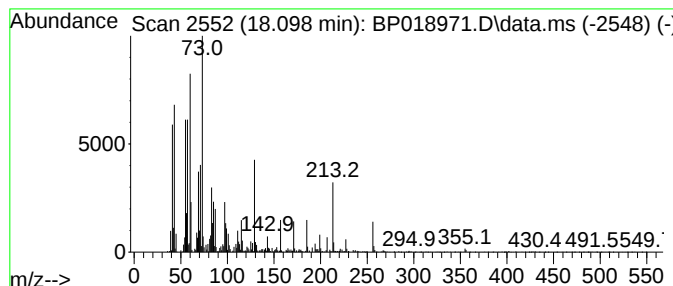
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	2.24 ng/ul	188518	Phenanthrene-d10	17.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96



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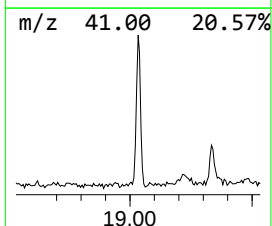
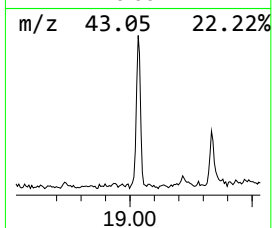
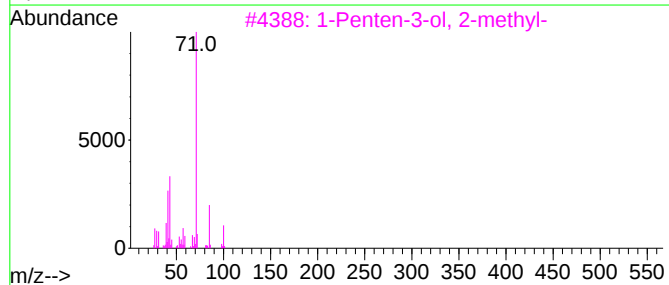
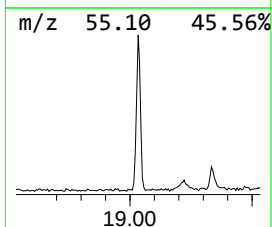
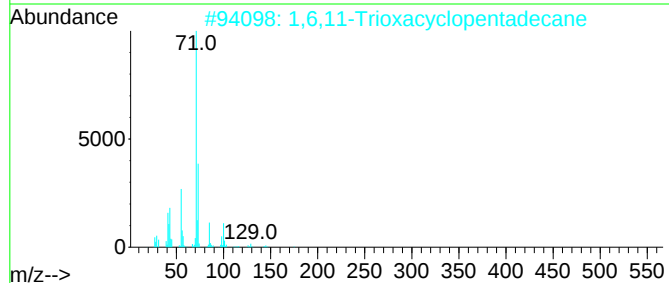
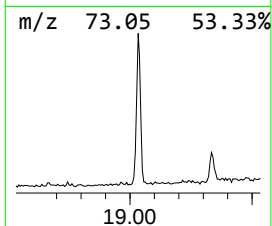
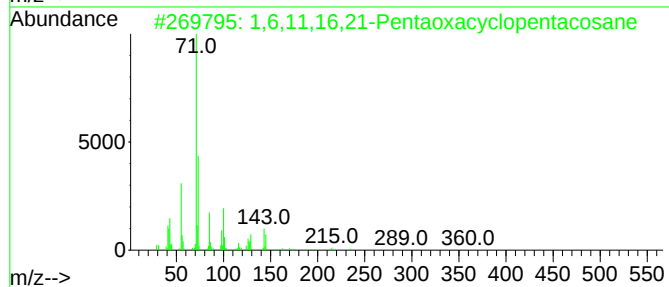
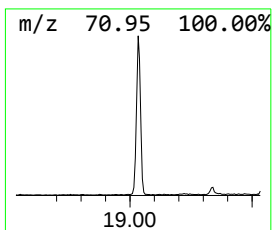
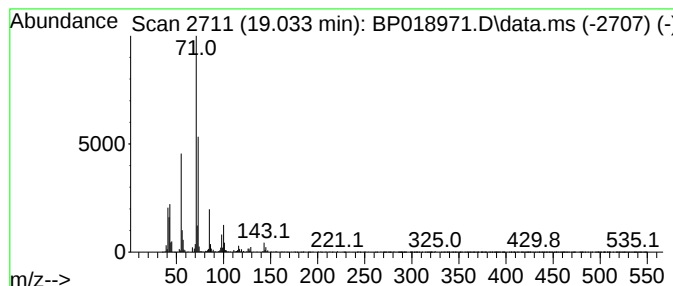
Instrument :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,6,11,16,21-Pentaoxacyclo... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.033	3.07 ng/ul	258266	Phenanthrene-d10	17.210	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	91
2	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	86
3	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	64
4	4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	50
5	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	50



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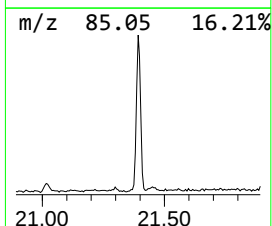
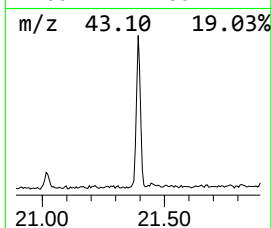
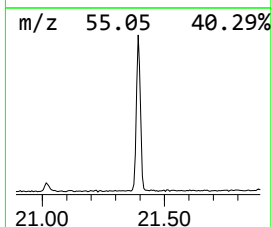
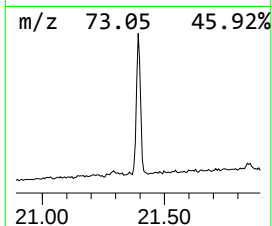
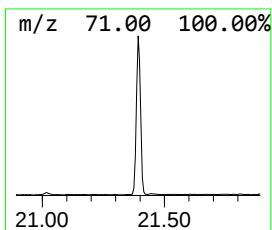
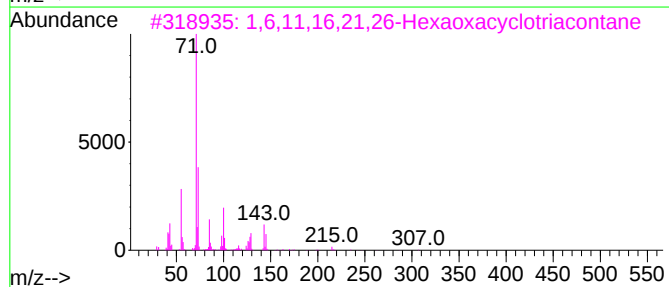
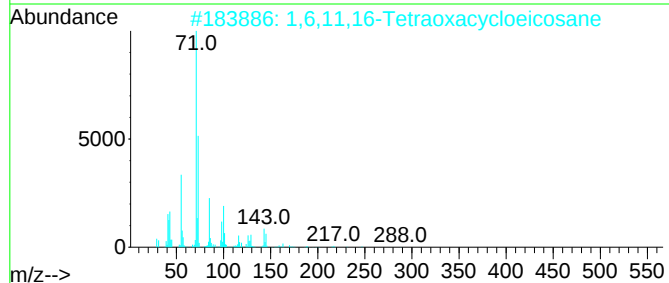
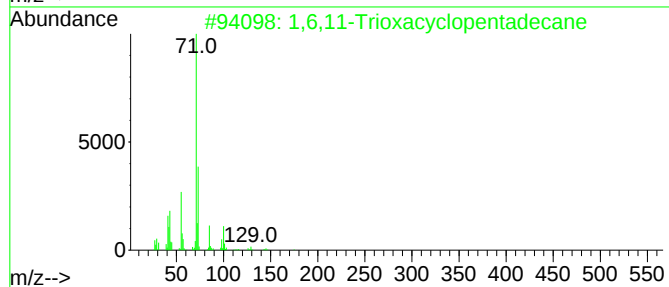
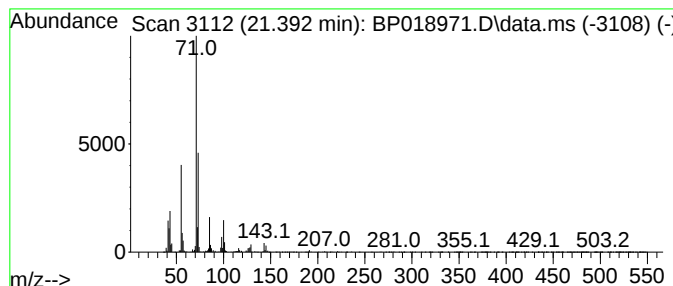
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TIC Library : C:\DATABASE\NIST20.L
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Peak Number 4 1,6,11-Trioxacyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.392	6.44 ng/ul	768741	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	86		
2	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	86		
3	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	86		
4	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	86		
5	./+/- Tetrahydro-3-furanmethanol	102	C5H10O2	015833-61-1	50		



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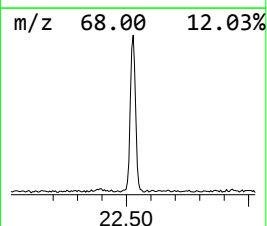
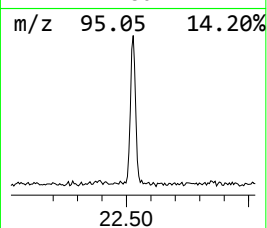
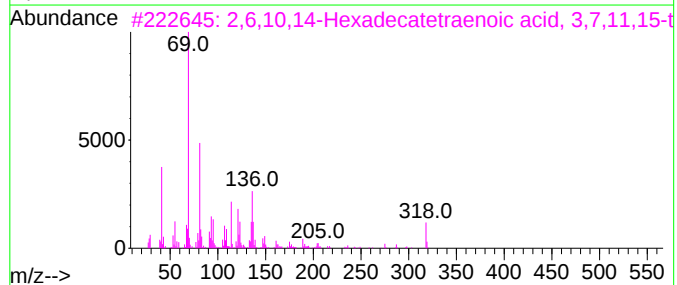
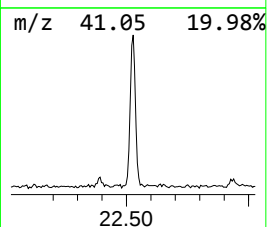
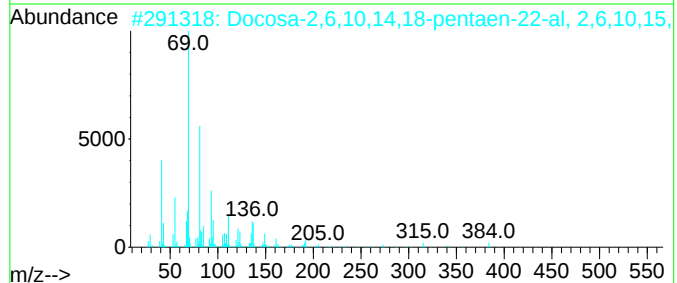
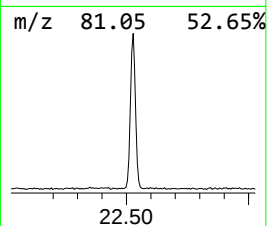
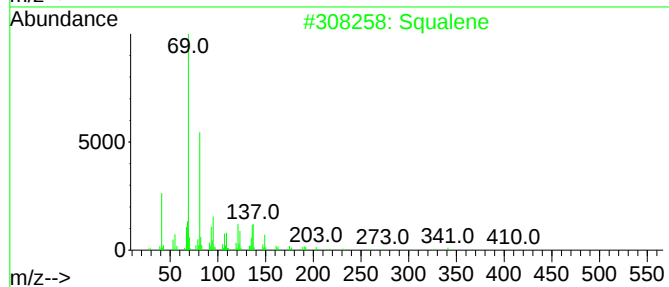
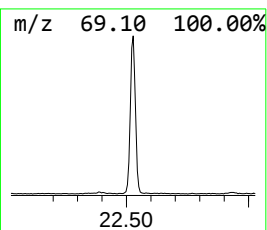
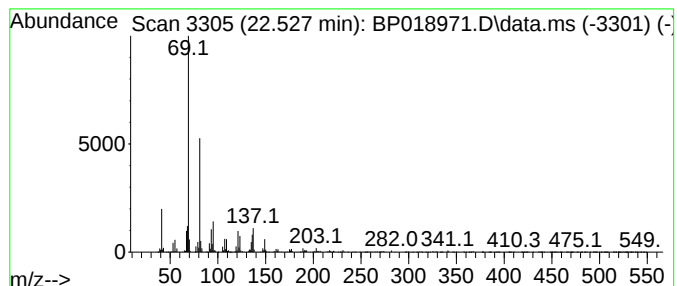
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.527	5.42 ng/ul	714008	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	89
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
3			2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	72
4			Farnesol isomer a	222	C15H26O	1000108-92-4	64
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



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ClientSampleId :
BH3K5

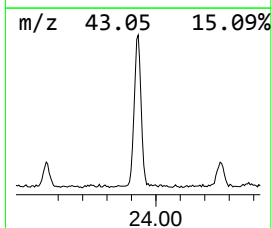
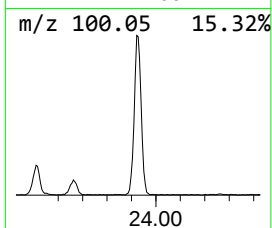
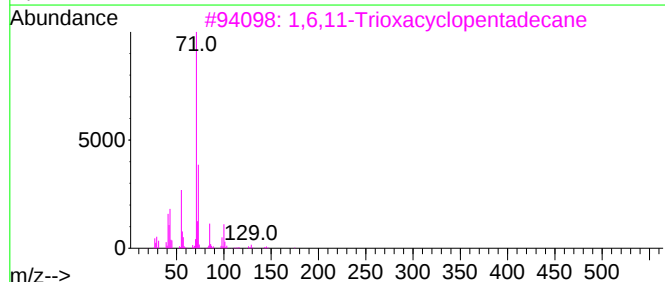
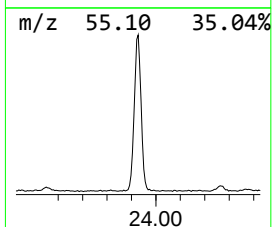
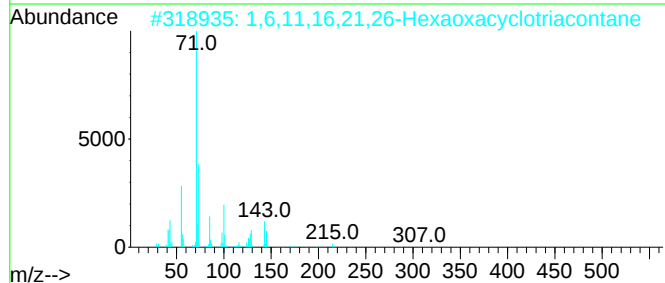
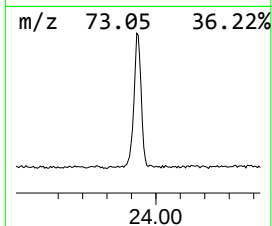
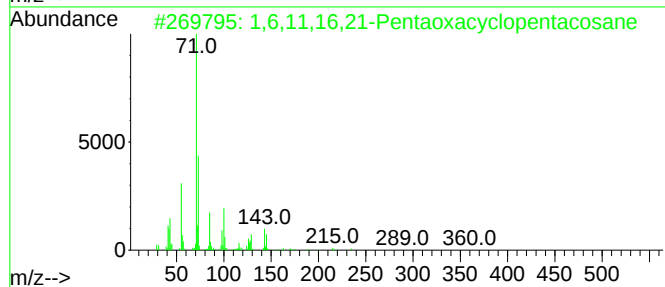
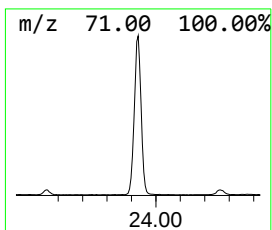
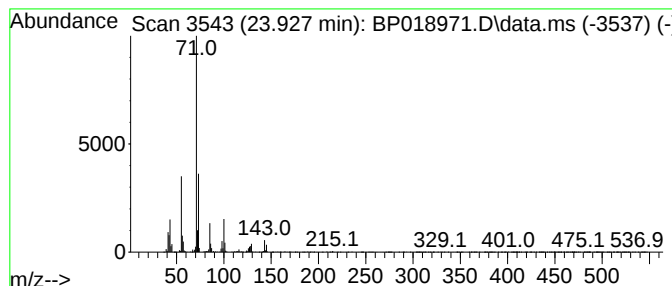
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.927	11.28 ng/ul	1484960	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H4005	056890-57-4	83		
2	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H4806	064001-05-4	64		
3	1,6,11-Trioxacyclopentadecane	216	C12H2403	000295-63-6	53		
4	Acrolein,dimethyl acetal	102	C5H1002	006044-68-4	47		
5	./+/-.-Tetrahydro-3-furanmethanol	102	C5H1002	015833-61-1	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
Data File : BP018971.D
Acq On : 20 Dec 2023 21:09
Operator : MA/JU
Sample : 05894-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BH3K5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzenesulfonam...	17.098	717.0	ng/ul	60299800	4	17.210	1682060	20.0
n-Hexadecanoic ...	18.098	2.2	ng/ul	188518	4	17.210	1682060	20.0
1,6,11,16,21-Pe...	19.033	3.1	ng/ul	258266	4	17.210	1682060	20.0
1,6,11-Trioxacy...	21.392	6.4	ng/ul	768741	5	21.298	2388890	20.0
Squalene	22.527	5.4	ng/ul	714008	6	23.663	2633580	20.0
1,6,11,16,21,26...	23.927	11.3	ng/ul	1484960	6	23.663	2633580	20.0